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Title of Submission

Computational cyberinfrastructure for advances in complex fluids: enabling the long tail of science

Abstract (maximum ~200 words).

Complex fluids appear everywhere in daily life (from polymers, to combustion to clouds to the medicines we take). Advances in computational algorithms and multiphysics modeling strategies have now opened up the possibility of in silico modeling, analysis and (more importantly) rational design of systems involving complex fluids. Most research groups involved in complex fluids require moderate yet sustained access to computational resources. This long tail of science is where a lot of creative ideas are being explored. We discuss this in the context of specific research examples within the broader arch of complex fluids (multiphase flows and polymer processing) where the dedicated availability of long term, moderate scale computational resources (100-500 cores for 48-96 hours) would yield dramatic results.

Question 1 Research Challenge(s) (maximum ~1200 words): Describe current or emerging science or engineering research challenge(s), providing context in terms of recent research activities and standing questions in the field.

We briefly describe some of the emerging research challenges and how the rapid availability of moderate computing resources can greatly accelerate research progress.

Understanding multiphase flow phenomena for energy and health care application: One of the outstanding problems in multiphase flows affecting a multitude of applications (combustion, fluidized beds, pharma operations) and natural phenomena (cloud formation) is the clustering of particles, droplets or bubbles in multiphase flows. This is a very challenging, inherently multiscale problem that can naturally take advantage of current progress in cyberinfrastructure, machine learning and data analytics. Broad open questions that the availability of cyber infrastructure can help tackle include (a) extending current mathematical descriptors of clustering (which are predominately first order statistics) to incorporate second and higher order statistics, and (b) utilizing simulation data of clustering at very fine resolution (but small investigation volumes) to construct closure models that can be used for simulations at low resolution (but large investigation volumes). This closure problem is a pressing problem in flow physics simulations where it is critical to build approximate representations of more complex fine-scale phenomena so as to be able to simulate phenomena of engineering relevance, and (c) dealing with the inherent uncertainty in such closure models using recently developed approaches (like Bayesian based approaches).

Several specific examples from energy and healthcare are as follows:
Energy and environment applications: The Energy Independence and Security Act (EISA) mandates blending of biofuels with the objective of reducing transportation sector emissions. Several technologies to produce biofuels involve fluidized beds, which are complex multi-scale systems to process biomasses, where fluid phases (gas or liquid) interact with the solid biomass and inert solid particles (i.e. sand, used to favor heat transfer) to perform chemical reactions, such as biomass gasification, combustion or conversion into biofuels. Similarly, several technologies for carbon capture also involve multiphase flows in fluidized beds. These include chemical looping combustion, second-generation carbon capture processes such as calcium looping, The design and optimization of fluidized systems are not trivial, and the physical phenomena that happen in them are not completely understood. For example, the interaction of the flow with particles affects the segregation of particles in the device, leading to formations of particle clusters, and, consequently, the heat and mass transfer, and the process yield. The complexity of the problem is exacerbated by the coupling of fluid mechanics and chemical reactions, which typically involves complex kinetic mechanisms. Research groups at ISU are developing a multi-scale paradigm to efficiently model this system that integrates particle resolved direct numerical simulations (PR-DNS) at the micro-scale with a multiphase model at the macro-scale.

Healthcare application: Functional nanoparticles are being extensively used as carriers for drug delivery, due to their capability of penetrating cellular walls, and to be functionalized to selectively target only the affected cells. One of the most advanced processes to produce nanoparticles of precisely controlled size is flash nanoprecipitation (FNP), which requires fast mixing of two or more streams to create supersaturation. A dissolved solute and a stabilizing amphiphilic polymer are rapidly mixed with an anti-solvent to create high supersaturation over a time scale shorter than the characteristic nucleation and growth time scales for the nanoparticles. The process also provides the capability to coat and create composite multi-functional particles, with precisely controlled particle size distribution. To understand this system, advanced computational models must be developed to describe the kinetics of precipitation, growth and aggregation of nanoparticles. These models account for the complex turbulent nature of the flow, the chemical kinetics, and the kinetics of nucleation, growth and aggregation of the nanoparticles.

Cardiovascular fluid structure interaction and optimization: Patient specific modeling can result in the development of personalized and effective healthcare treatments. As an example, groups at Iowa State university are developing the next generation of predictive simulation methods and tools for fluid–structure interaction (FSI) problems, with significantly improved representation of complex geometric designs and multi-physics phenomena. This has broad applicability (for instance, gas turbine efficiency), with specific focus on FSI design optimization for improving artificial heart valve durability. The challenges are to develop accurate, robust, and efficient design-through-analysis frameworks, that will enable rapid patient-specific designs of heart valves. Given the multi-physics nature of the problems, as well as the length and time scales involved, HPC is viewed as an indispensable technology for obtaining high-fidelity simulation results.

Computationally exploring process-structure-property for the rational design of designer materials and coatings: Conducting polymers exhibit a variety of properties (flexibility, tenability, easy processability) that make them a very promising material for a variety of critical technologies like bioelectronics, membranes, skin-compatible sensors, as well as consumer electronics. It is known that the final morphology of the active layer of organic electronic devices critically affects performance and reliability. Thus, tailoring the morphology is a key criterion in optimizing performance. A major hindrance to efficient design of high performance devices is identification of promising fabricating conditions out of innumerable possibilities. This includes composition and processing conditions (fabrication process – spin coating, inkjet printing, drop casting – that impact fluid stresses, solvent type, nature of substrates, presence of additives), post fabrication annealing, and encapsulation. Experimentally exploring these infinite possibilities is infeasible. A variety of research groups at ISU have been developing and disseminating virtual manufacturing workflows that will enable high throughput exploration of various processing pathways. This multidisciplinary group of engineers and data scientists is pursuing fundamental research to provide needed knowledge to understand morphology formation using a multiscale theoretical approach. This research integrates first principles and molecular methods with meso-scale continuum methods to create a cohesive, atomistic-continuum framework that will require HPC resources to execute. A data driven approach to sampling the processing space will allow knowledge discovery via pattern recognition and hierarchical learning. The results from this research will have broad applicability across a diverse spectrum of technologies, such as solar cells, diode lighting, flexible displays, and bioelectronics, thus directly benefiting the U.S. economy and society.

Question 2 Cyberinfrastructure Needed to Address the Research Challenge(s) (maximum ~1200 words): Describe any limitations or absence of existing cyberinfrastructure, and/or specific technical advancements in cyberinfrastructure (e.g. advanced computing, data infrastructure, software infrastructure, applications, networking, cybersecurity), that must be addressed to accomplish the identified research challenge(s).

Most of the computational approaches used to investigate problems concerning these applications are moderately computationally intensive (100-500 CPUs), but need to be executed for long period of times (few days), due to the transient nature of the phenomena that are being investigated. Scientific investigations will then involve several cases to be examined (of the order of 10 to 1000), which will need to be run for periods up to 96 hours, generating moderately large amout of data, which will be either analyzed on the fly during the simulation, or a-posteriori, but always on the HPC machine, due to the size of datasets. An infrastructure capable of accommodating these needs, without significant wait times, would enable scientists to accelerate their investigations and increase the turnaround time to produce applicable results in their areas.

While TACC Stampede and SDSC Comet have been exceptional resources; in the recent year wait times for access to compute nodes on these resources is of the order of days (2-3 days) making computational research quite frustrating. This is indicative of the increasing utilization of these machines (with frequent over subscription), thus warranting further increase and availability of XSEDE resources.

An alternative is to identify additional XSEDE partners (especially in the Midwest) that can host large scale infrastructure to enable the long chain of science access to such infrastructure.